

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

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1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE Technical Papers	3. DATES COVERED (From - To)		
4. TITLE AND SUBTITLE		5a. CONTRACT NUMBER		
		5b. GRANT NUMBER		
		5c. PROGRAM ELEMENT NUMBER		
6. AUTHOR(S)		5d. PROJECT NUMBER 2303		
		5e. TASK NUMBER M2C8		
		5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)		8. PERFORMING ORGANIZATION REPORT		
Air Force Research Laboratory (AFMC) AFRL/PRS 5 Pollux Drive Edwards AFB CA 93524-7048				
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)		
Air Force Research Laboratory (AFMC) AFRL/PRS 5 Pollux Drive Edwards AFB CA 93524-7048		11. SPONSOR/MONITOR'S NUMBER(S)		
12. DISTRIBUTION / AVAILABILITY STATEMENT				
Approved for public release; distribution unlimited.				
13. SUPPLEMENTARY NOTES				
14. ABSTRACT				
15. SUBJECT TERMS				
16. SECURITY CLASSIFICATION OF:		17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Leilani Richardson
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified	A	19b. TELEPHONE NUMBER (include area code) (661) 275-5015

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Separate items are enclosed

~~DDR&COO~~
2303 M2C8

TP-FY99-0162

✓ DTS

MEMORANDUM FOR PRS (Contractor/In-House Publication)

FROM: PROI (TI) (STINFO)

2 July 1999

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-TP-FY99-0162
Dr Perkins, "Computational Chemistry and Material Science for Rocket Propulsion"

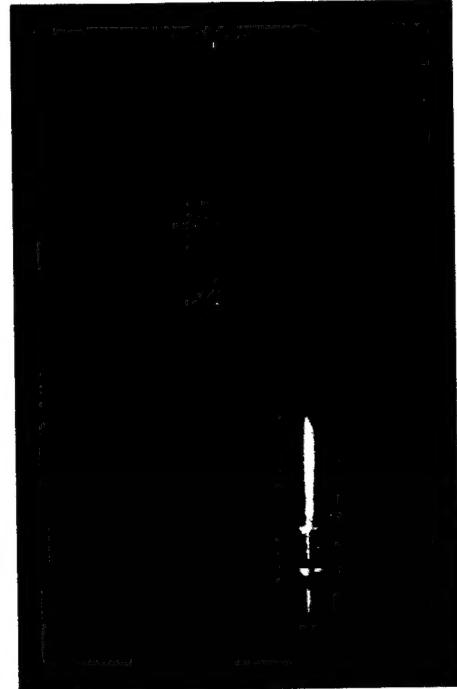
Defense S&T Presentation

(Statement A)

Computational Chemistry and Materials Science for Rocket Propulsion



20021121 014



Dr. Leslie S. Perkins
Propulsion Directorate
Air Force Research Lab
Edwards AFB CA 93524

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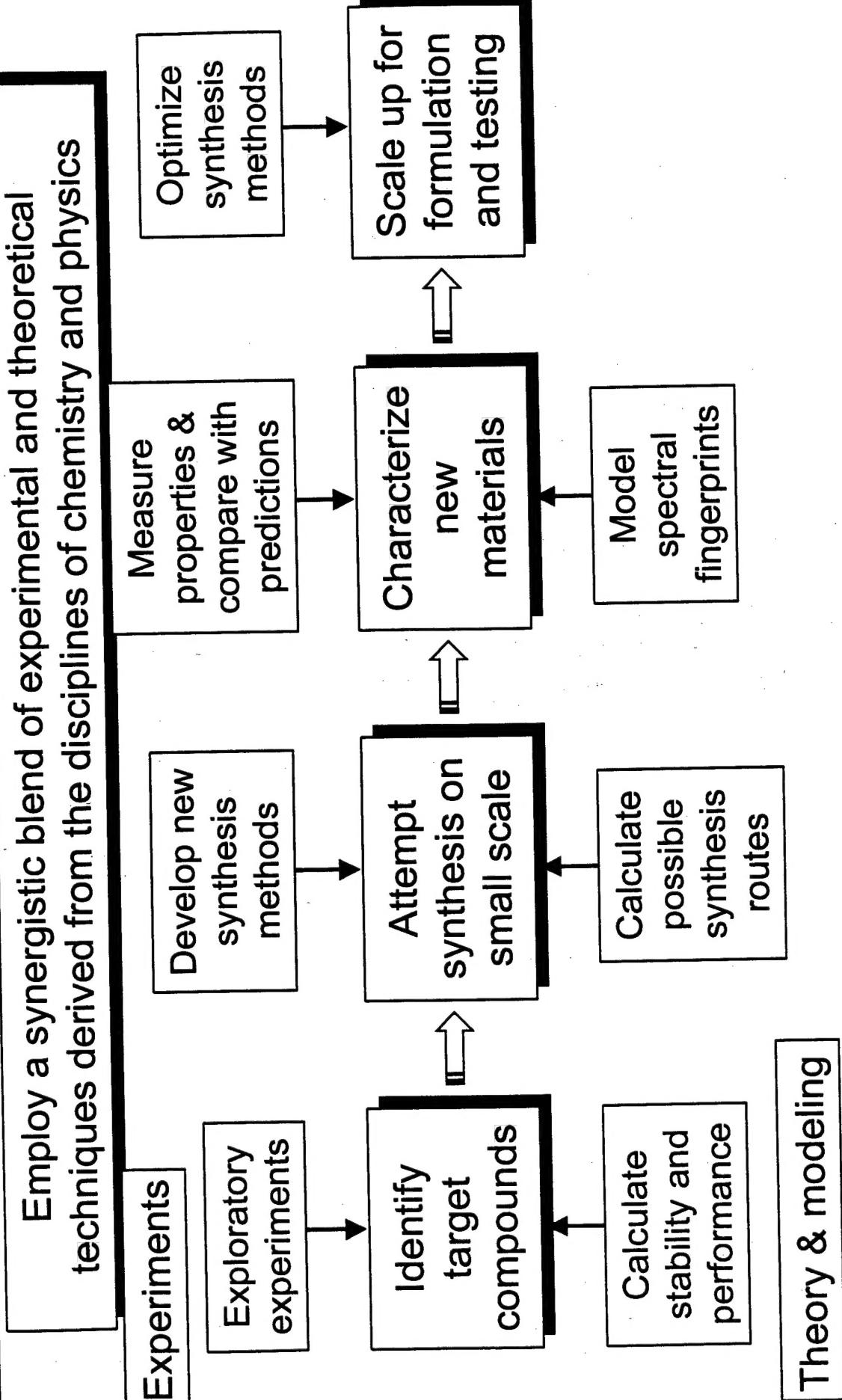
High Performance Computing is Vital to Materials Development in Rocket Propulsion!



- Identifies material improvements for liquid engines and solid motors
- Decide which proposed materials are worthwhile to pursue: Months rather than years!
- Reduces the long process to synthesize new materials.
- Eliminate unlikely pathways for making a new material



Approach to Developing Advanced Materials



New Energetic All-Nitrogen Compound

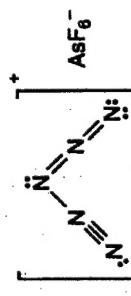


From *Chemical and Engineering News*, 25 Jan 99

news of the week

N₅⁺ CATION MAKES EXPLOSIVE DEBUT

High-energy ion is first new
all-nitrogen species in 100 years



It wasn't in his abstract, but Karl O. Christe, a chemist who studies high-energy materials at the Air Force Research Laboratory at Edwards Air Force Base in California, had a little something extra to offer last week in his plenary presentation at the American Chemical Society's Winter Fluorine Conference in St. Petersburg Beach, Fla. Along with colleague William W. Wilson, Christe has synthesized and characterized a salt containing the N_5^+ cation. The cation is the first new all-nitrogen species to be synthesized in isolable quantities in more than a century, and only the third ever to be produced. Although species that contain only ni-

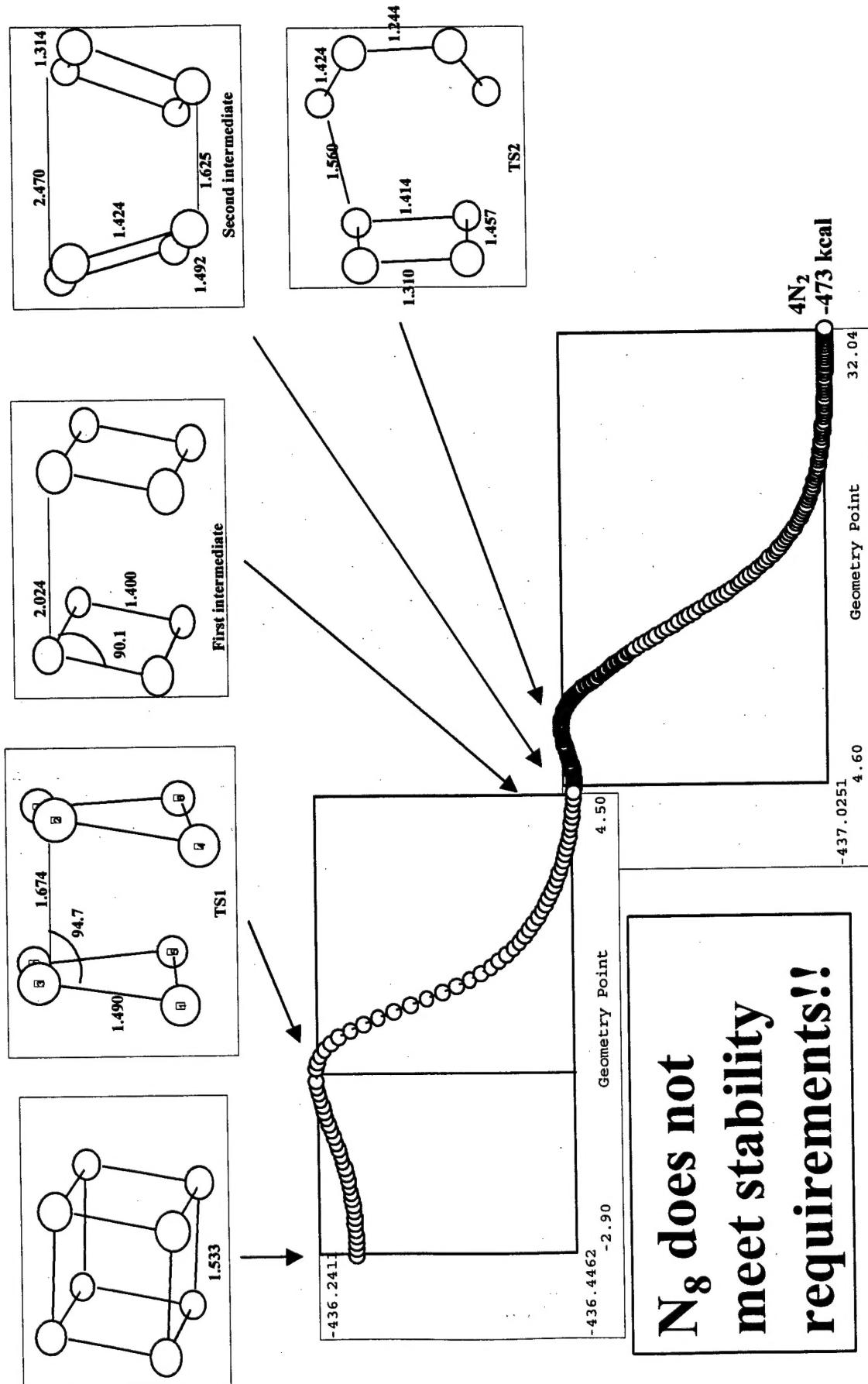
"The theoretical critics who are 'many' most interested in the new cation. "It's going to be of incredible interest to theoreticians who, perhaps, thought that compounds like this would be too unstable to isolate at all," Strauss says.

The salt is surprisingly stable, considering its huge calculated positive heat of formation of more than 350 kcal per mol. Christe points out. Vibrational spectroscopy and theoretical calculations by his coworkers Jeffrey A. Sheehy and Jerry A. Boatz show the cation to have a V shape in which resonance structures in

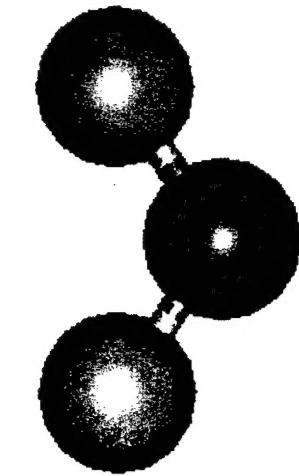
Clarke and his group envision other N_5^+ salts—such as $N_5^+SbF_6^-$ —that might have even more thermal stability. They also would like to use the cation to pre-



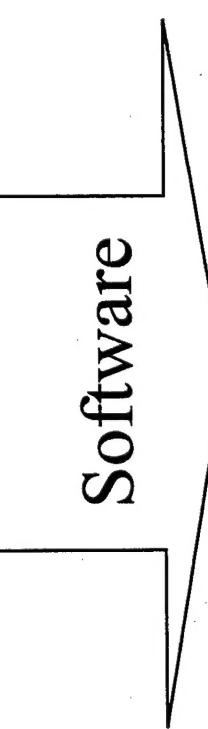
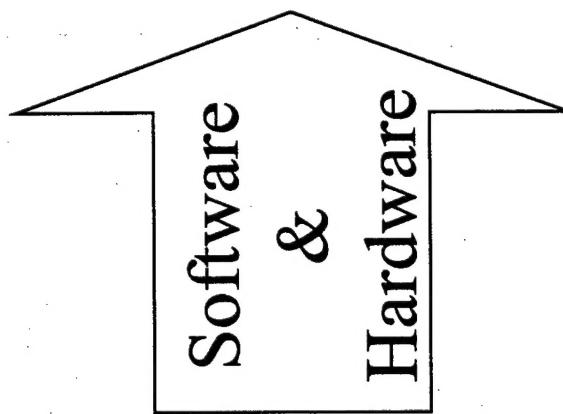
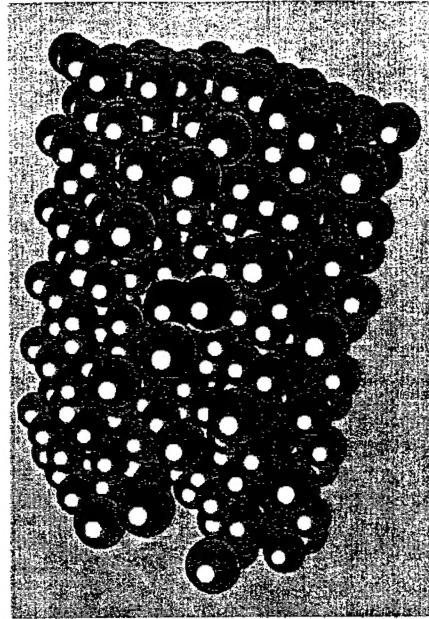
Evaluation of N_8 for stability



HPC aids in identifying future propellants



In 1987, a single calculation would take over 1 week.



GAMESS calculation on a workstation: 8 hours!!

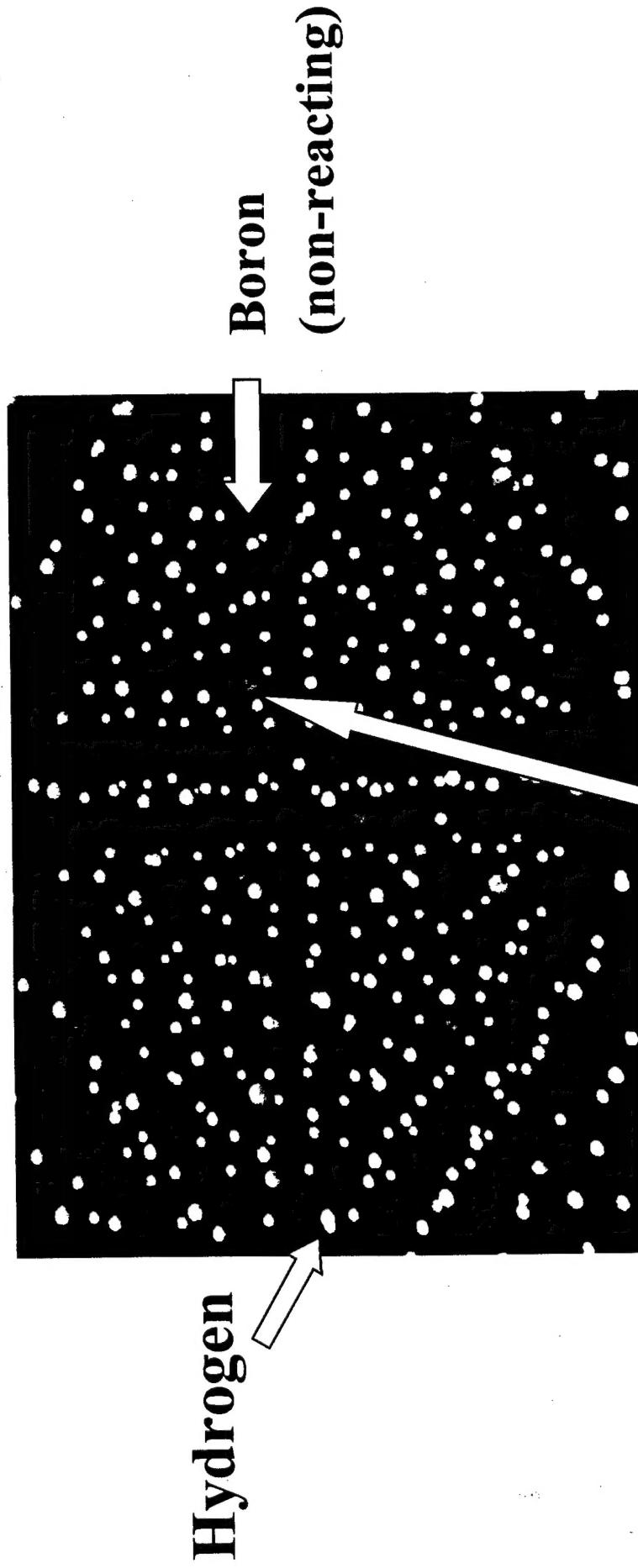
B in *para*-H₂: 200 times the number of atoms in 5 weeks on IBM SP!! (This would require 4 YEARS on a workstation)

Future Solid Propellants



6.25% boron atoms in solid *para*-hydrogen

(64 nodes on an IBM SP at Maui - 5 weeks)



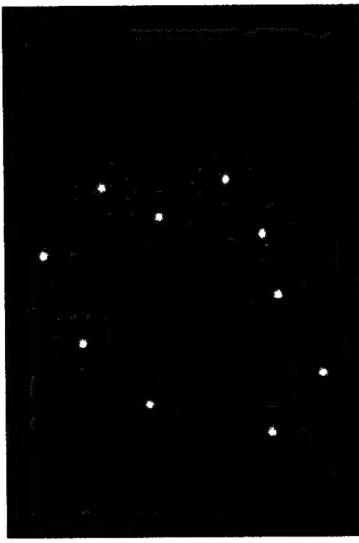
Boron (reacting)

After reaction: Only local recombination of impurities!



CMID: Quantum Particles and Classical Dynamics

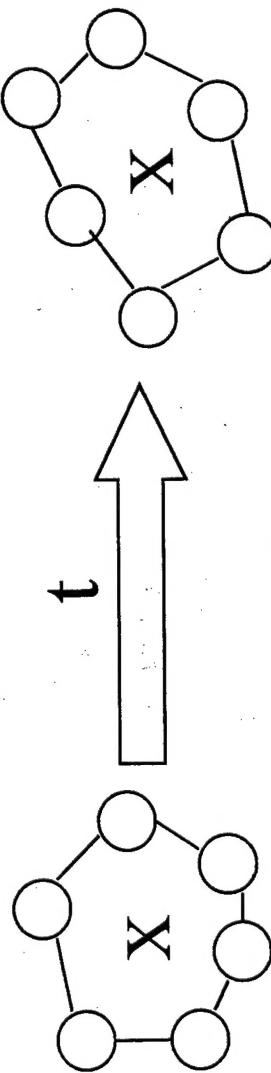
1. Treat the quantum particles as a “ring” of classical particles



Quantum $\propto M^N$

Classical $\propto N$ to N^2

2. The dynamics of the “ring” is calculated for each time step.



$q_c(0)$ $q_c(t)$



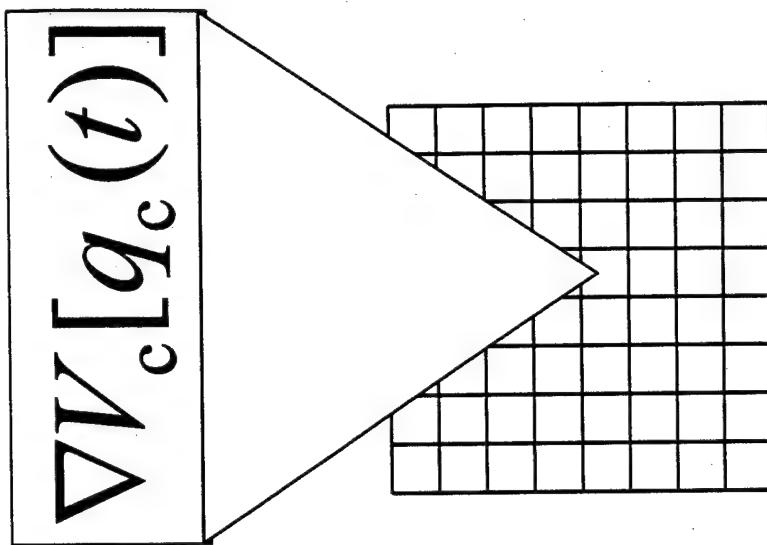
CMID on HPC Architectures

Compute the movement of particles using:

$$m \bullet \frac{d^2 q_c(t)}{dt^2} = -\vec{\nabla} V_c[q_c(t)]$$

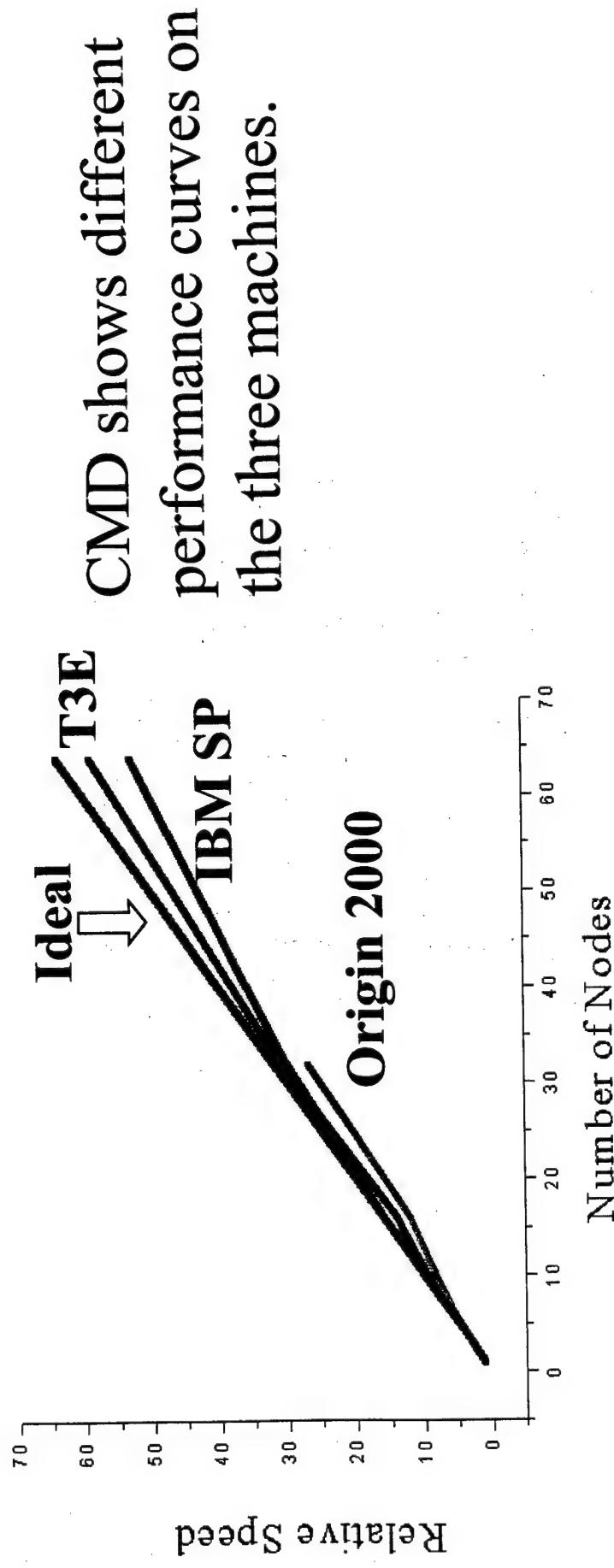
where

$$V_c(q_c) = -k_B T \ln[\rho_c(q_c)]$$



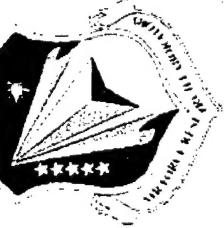
The largest part of the work is solution of the forces. It is equally balanced onto 64 nodes.

How does CMD perform on HPC machines?

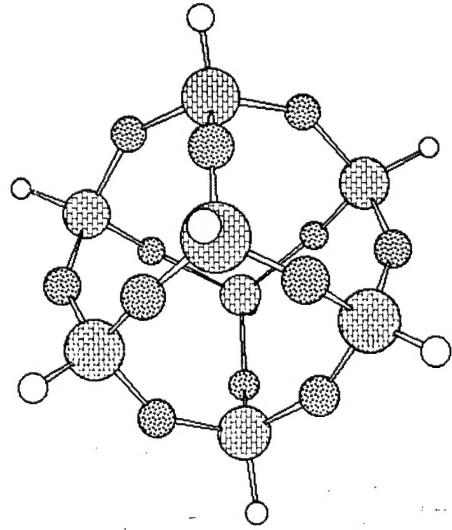


CMD shows different performance curves on the three machines.

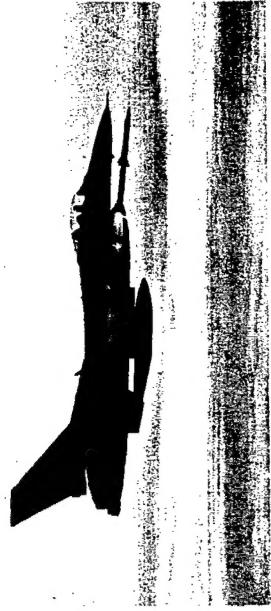
Parallel coding is not a “one-size fits all” procedure



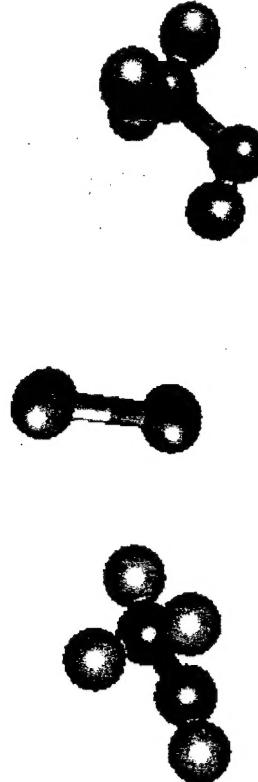
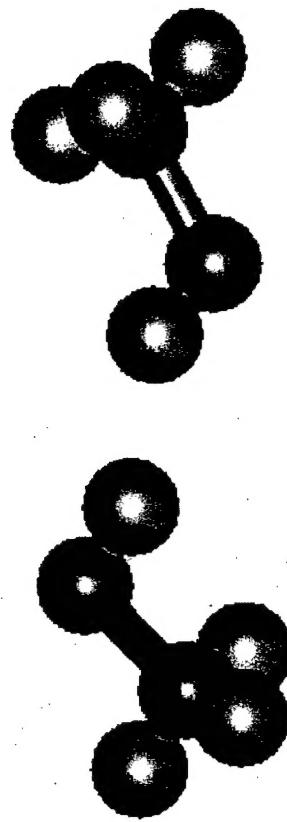
HPC in Materials Design and Synthesis



Polyhedral
Oligomeric
Silsesquioxane
(POSS)



Significant barrier to
initial condensation -
20 kcal/mol

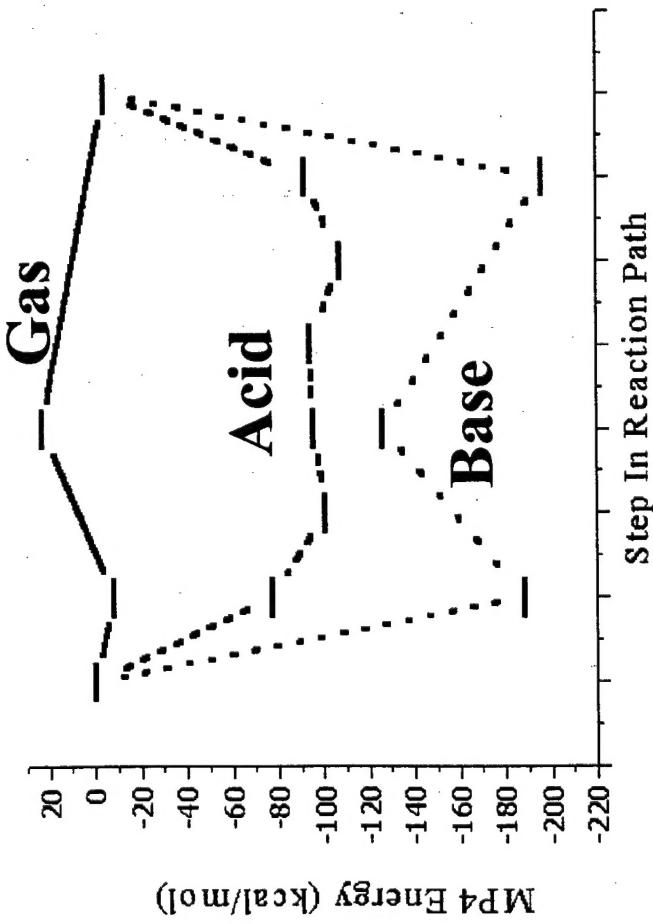


In a basic solution, the
condensation pathway is
more favorable!

Condensation of POSS



- There are different reaction pathways with different liquid environments
- Aids in experimental design to get to end product
- UNABLE to accomplish prior to HPC!!



Computational Chemistry and Materials Science - Future Directions



- Simulations of "real" sized systems
 - Material simulations consisting of billions of atoms with a volume of *at least* 1 cubic centimeter
- Dynamic and static simulations that include ~~a~~ quantum effects *without* a significant turnaround time for results
- Software development that incorporates quantum mechanics in an ingenious manner

HPC - What has it done for Rocket Propulsion?



- HPC has identified likely candidates (N_5^+ , B in solid H, POSS) and rejected unlikely prospects (H_4, N_8) in the AFRL/PR Rocket Propellant and Rocket Component Materials programs
- HPC has identified likely routes to achieve the creation of new rocket materials